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MEMORANDUM FOR PRR (~~Contractor~~/In-House Publication)

2 June1999

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Jeff Mills, "Hydrocarbon Fuels Optimization"
Poster Session – HEDM Conference **(Public Release)**

Hydrocarbon Fuels Optimization

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Introduction–

Hydrocarbon fuels, as a class, are investigated using the minimal set of parameters determinative of oxidizer-optimized specific impulse and common density-specific-impulse analogues. In this context specific families of promising candidate fuels can be systematically compared, the performance trade-offs among the relevant chemical and physical properties can be quantified, and the general characteristics of mission-tailored fuels can begin to be elucidated.

Initial Questions–

- Why do I sometimes get relatively poor theoretical ? performance from a high-energy hydrocarbon?
- Why is RP-1 (kerosene) such a good rocket fuel?
- What are the minimal set of fuel parameters that determine hydrocarbon I_{sp}?
- What are the performance trade-offs among these parameters?
- How can I begin to use this information to search for the "optimum" hydrocarbon fuel and reduce "hunt and peck" methods?

General Concepts/Initial Approximations–

Characteristics of "Good" Rocket Fuels:

- **High Heat of Formation**
- **High "Light-Atom" Content**

Specific Impulse:

(Momentum Transfer from Combusted Ejecta)

For an optimal nozzle:

$$I_{sp} \equiv \frac{1}{g}\sqrt{2\,(H_{chamb.} - H_{exh.})}$$

Sometimes approximated:

$$(I_{sp})_{opt} \propto \frac{1}{g}\sqrt{2\,\Delta H_{comb.}}$$

or,

$$(I_{sp})_{opt} \propto \frac{1}{g}\sqrt{2\,\Delta H_{f}}$$

ΔH_{comb}–stoichiometric combustion enthalpy

(per unit mass of exhaust products)

ΔH_{f}–specific enthalpy of formation

More Realistic Model Rocket–

One-Dimensional, Adiabatic, Equilibrated, Isentropic Expansion from the Combustion Chamber

Reference Rocket Conditions for I_{sp} Optimized vs. LOX:

Sea level expansion:

$$P_{chamber} = 1000 \text{ psi}, \; P_{exhaust} = 14.7 \text{ psi}$$

"Vacuum" expansion:

$$P_{chamber} = 1000 \text{ psi}, \; \epsilon = 40$$

Sole determinative parameters of LOX-optimized specific impulse and its density variants:

$$(I_{sp})_{opt} \Leftarrow \Delta H_f(/g) \text{ and } r\left(\frac{H}{C}\right)$$

$$(\rho_{of}^{a}\, I_{sp})_{opt} \Leftarrow \Delta H_f(/g),\ r\left(\frac{H}{C}\right),\ \rho_f,\ \text{and } a$$

$\Delta H_f(/g)$–specific enthalpy of formation of the fuel

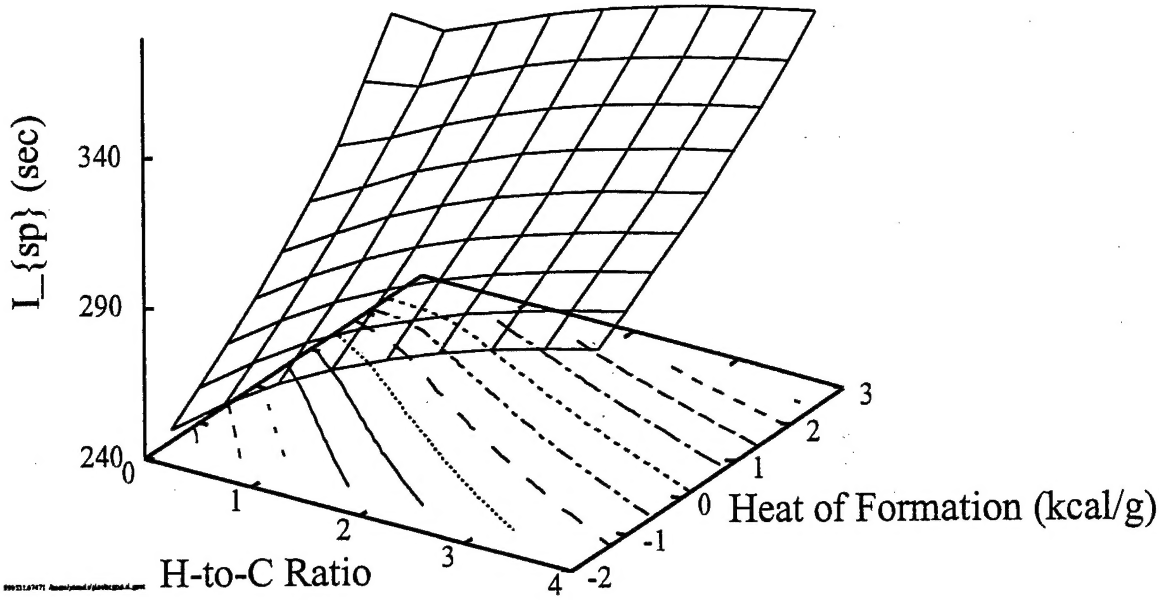
$r\left(\frac{H}{C}\right)$–atom ratio of fuel

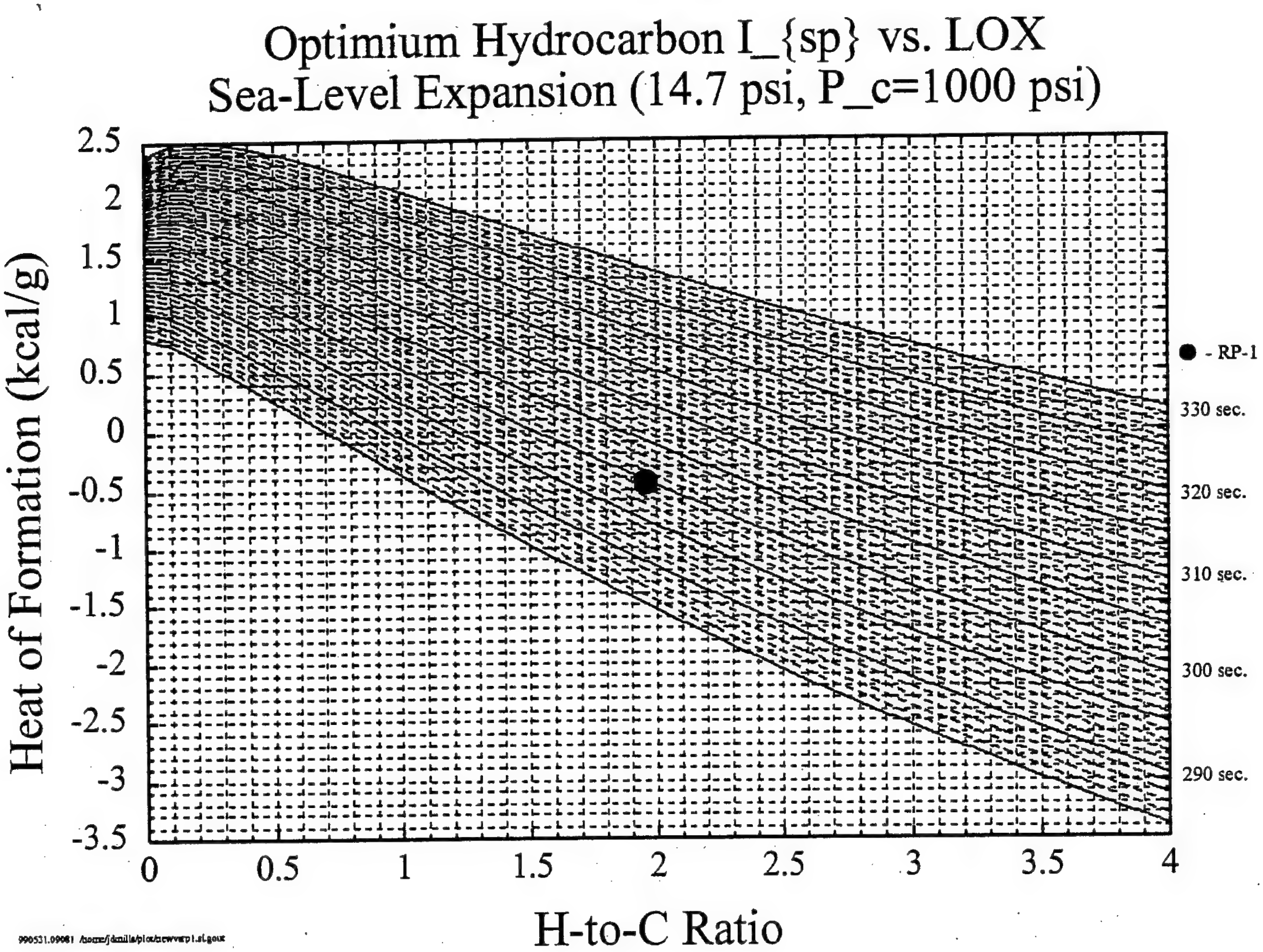
ρ_{of}–oxidizer-fuel bulk density

ρ_f–fuel density

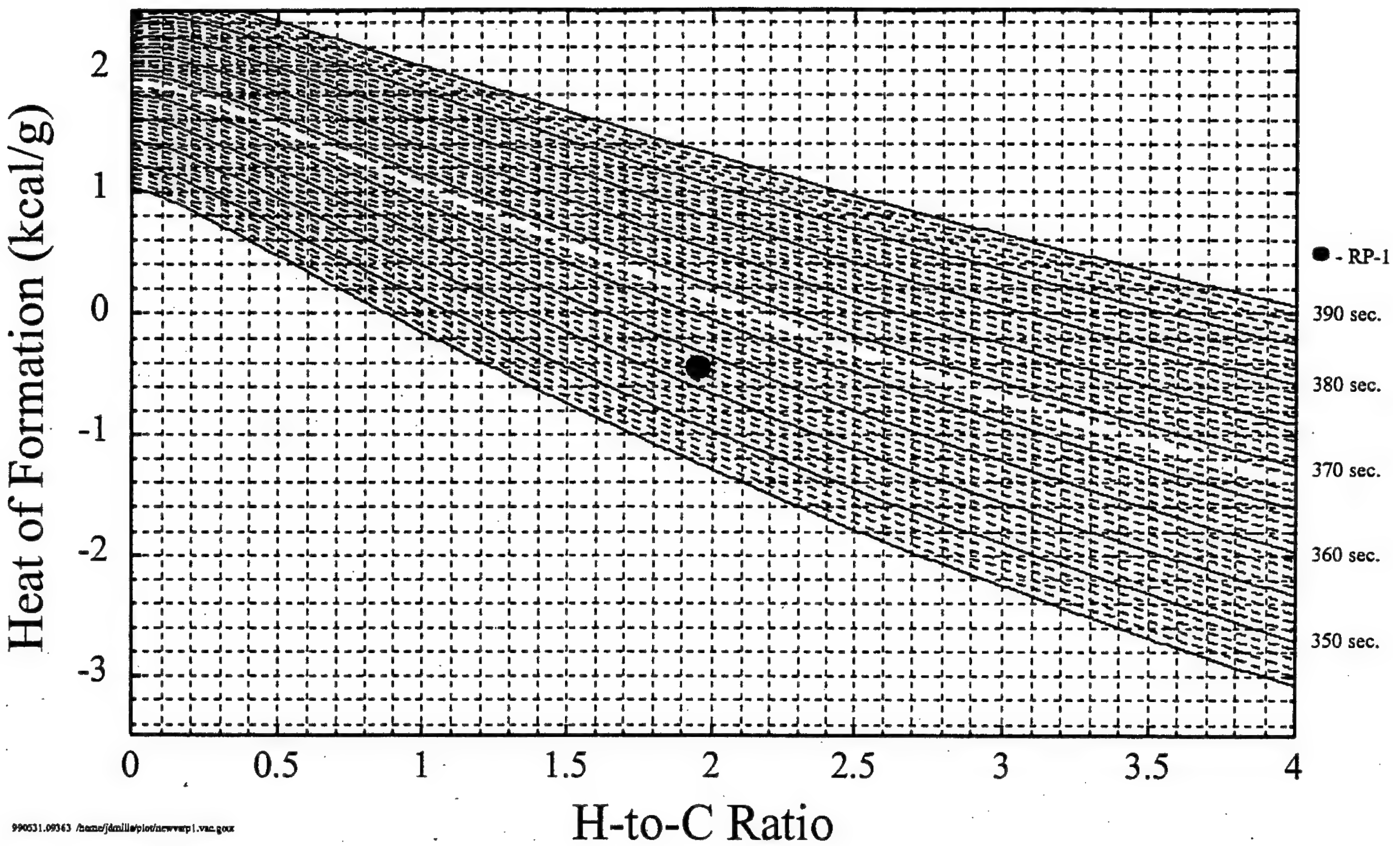
a–density exponent (often, mission-specific constant)

Optimium Hydrocarbon I_{sp} vs. LOX
Sea-Level Expansion (14.7 psi, P_c=1000 psi)




Optimium Hydrocarbon I_{sp} vs. LOX
Sea-Level Expansion (14.7 psi, P_c=1000 psi)
Heat of Formation (kcal/g)
2.5
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-2.5
-3
-3.5
0
0.5
1
1.5
2
2.5
3
3.5
4
H-to-C Ratio
● - RP-1
330 sec.
320 sec.
310 sec.
300 sec.
290 sec.

Optimium Hydrocarbon I_{sp} vs. LOX
Vacuum Expansion ({/Symbol e}=40, P_c=1000 psi)



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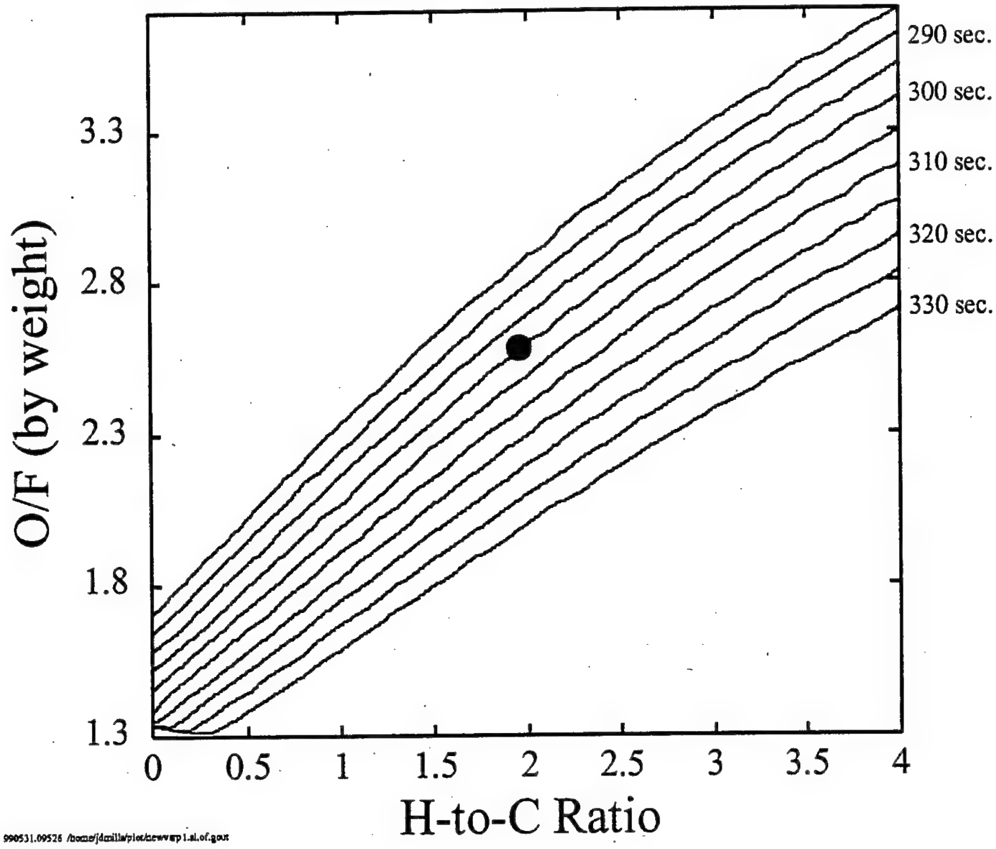
O/F at Optimium I_{sp}
Sea-Level Expansion (14.7 psi, P_c=1000 psi)



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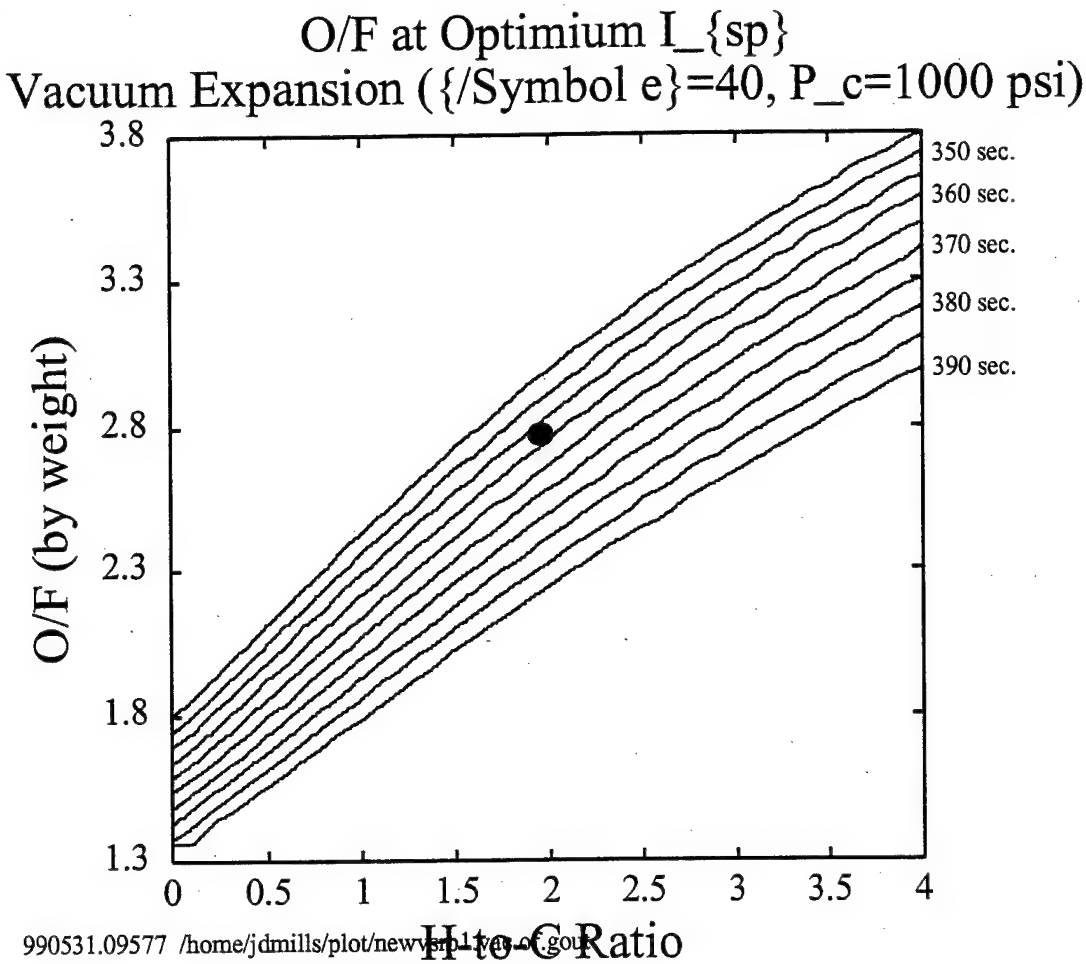

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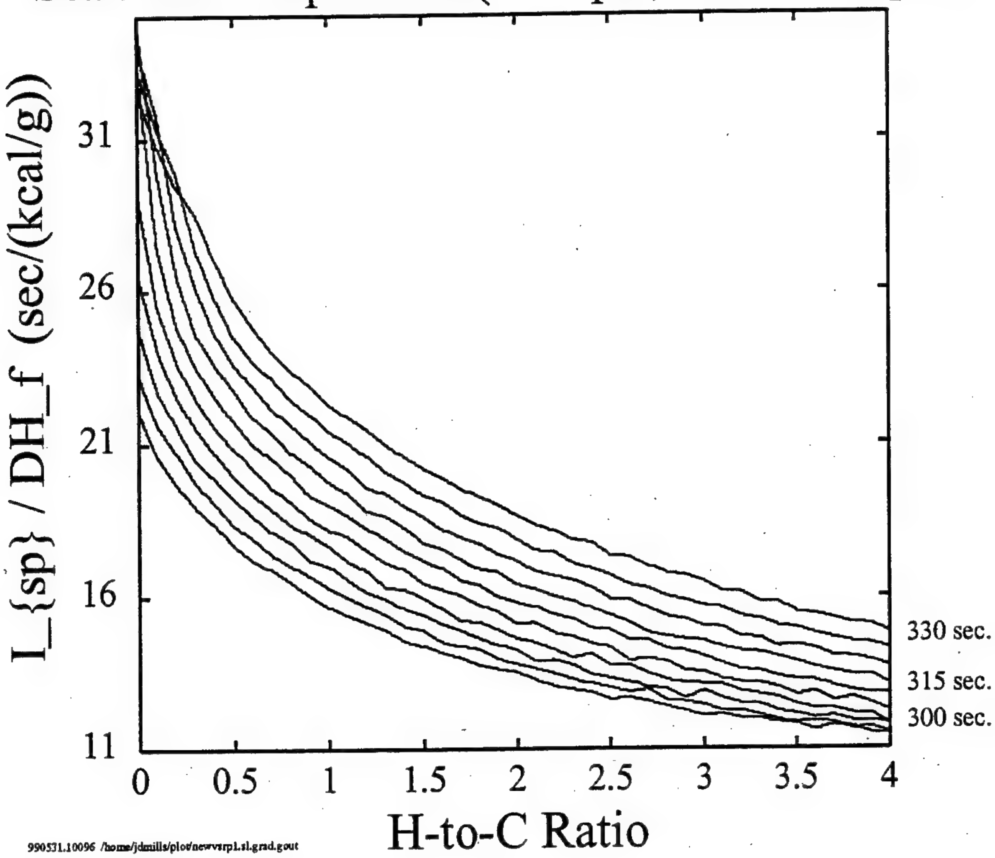
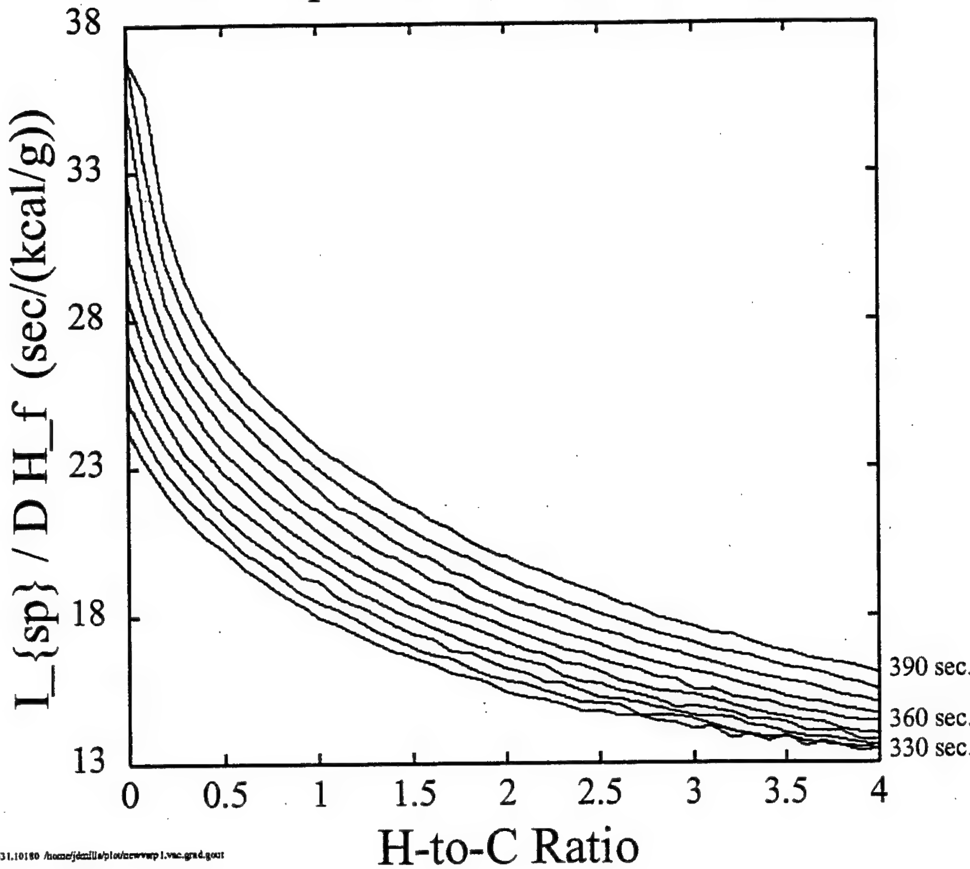
Errors in Optimium I_{sp} with D H_f
Sea-Level Expansion (14.7 psi, P_c=1000 psi)



Errors in Optimium I_{sp} with D H_f
Vacuum Expansion (e=40, P_c=1000 psi)



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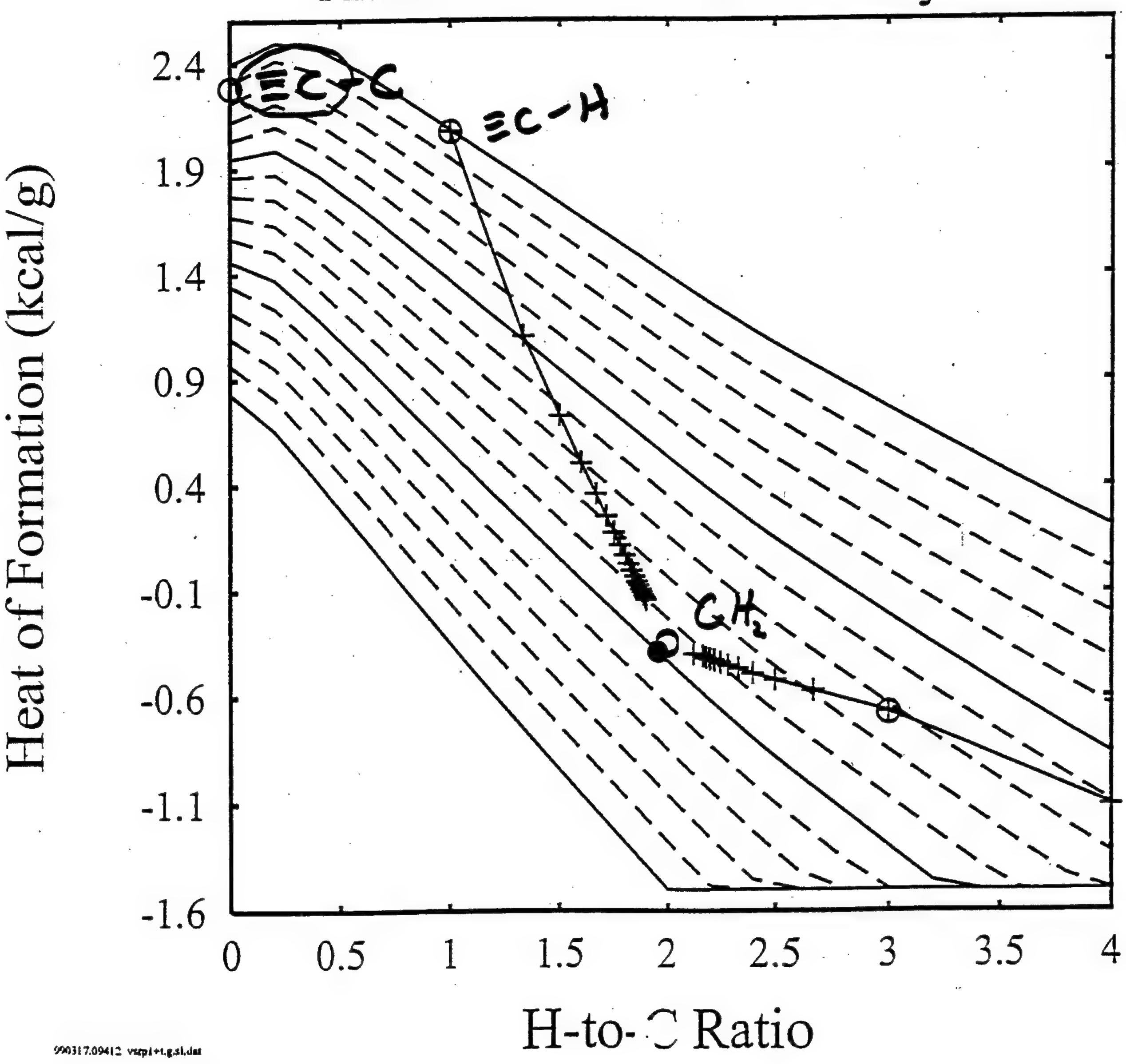
A Specific-Impulse Survey of Chemical Families–

Gas, Sea-Level Hydrocarbon Performance
Alkanes and Terminal Alkynes



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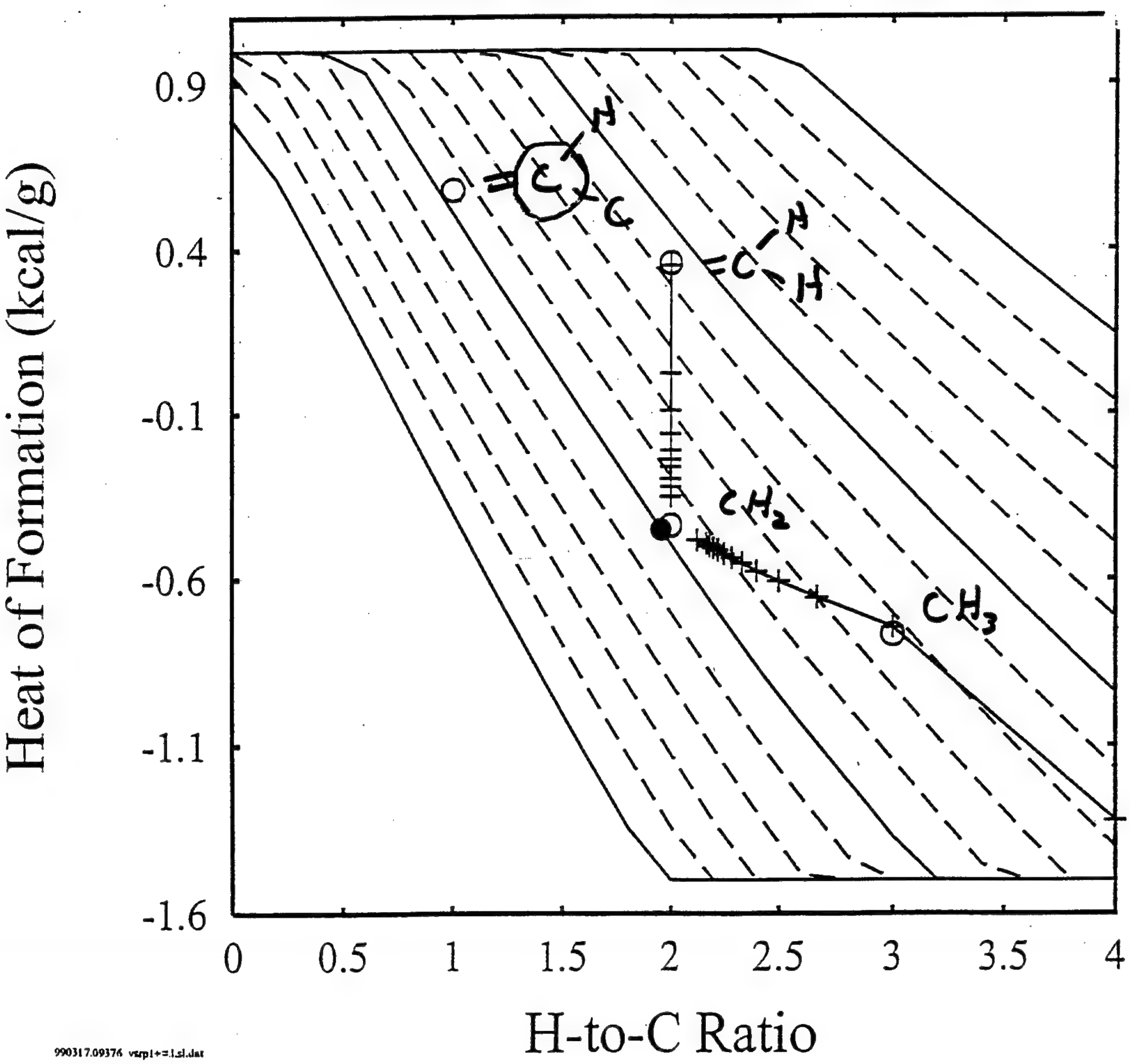
Liquid, Sea-Level Hydrocarbon Performance
Alkanes and Terminal Alkenes



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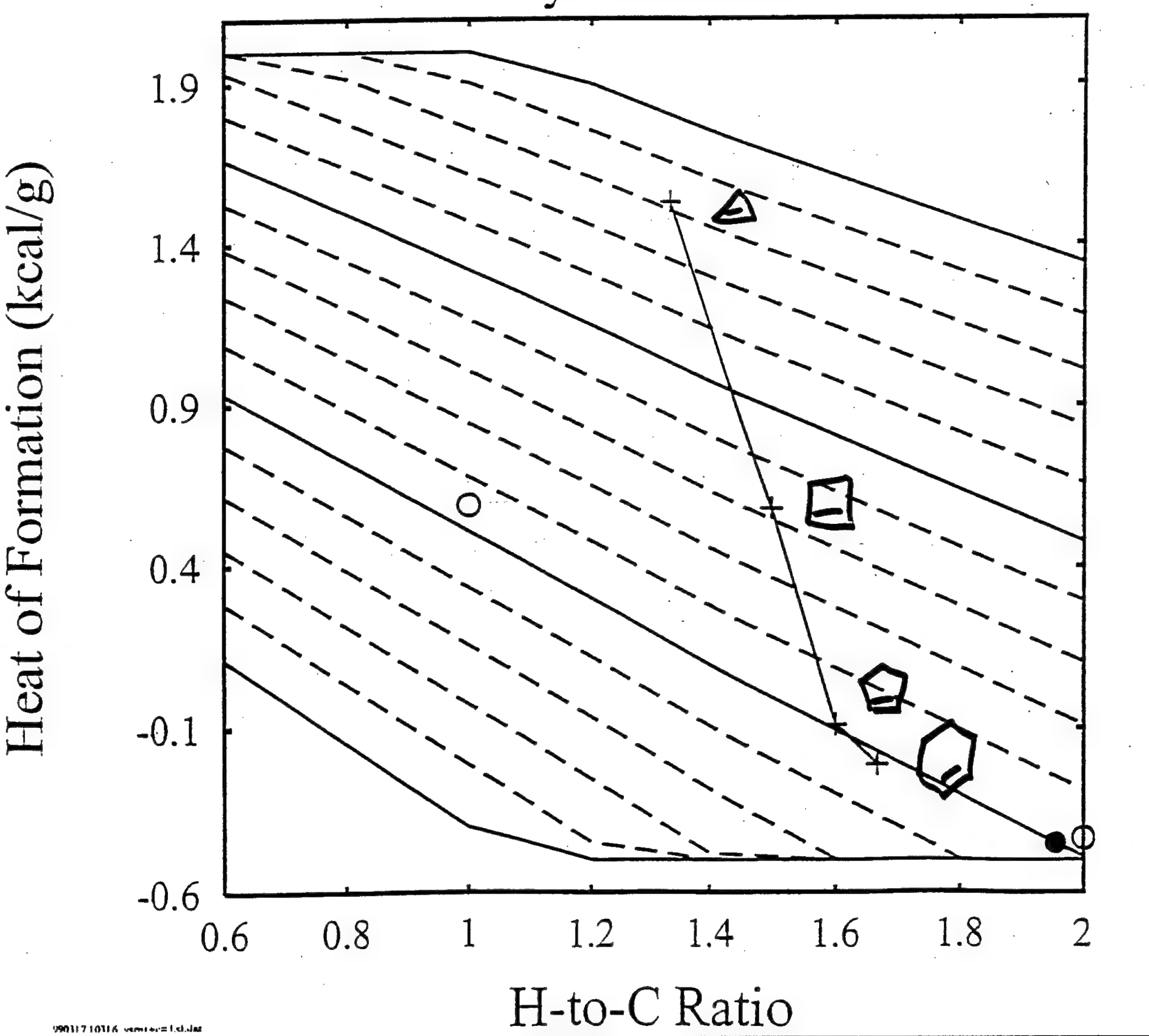
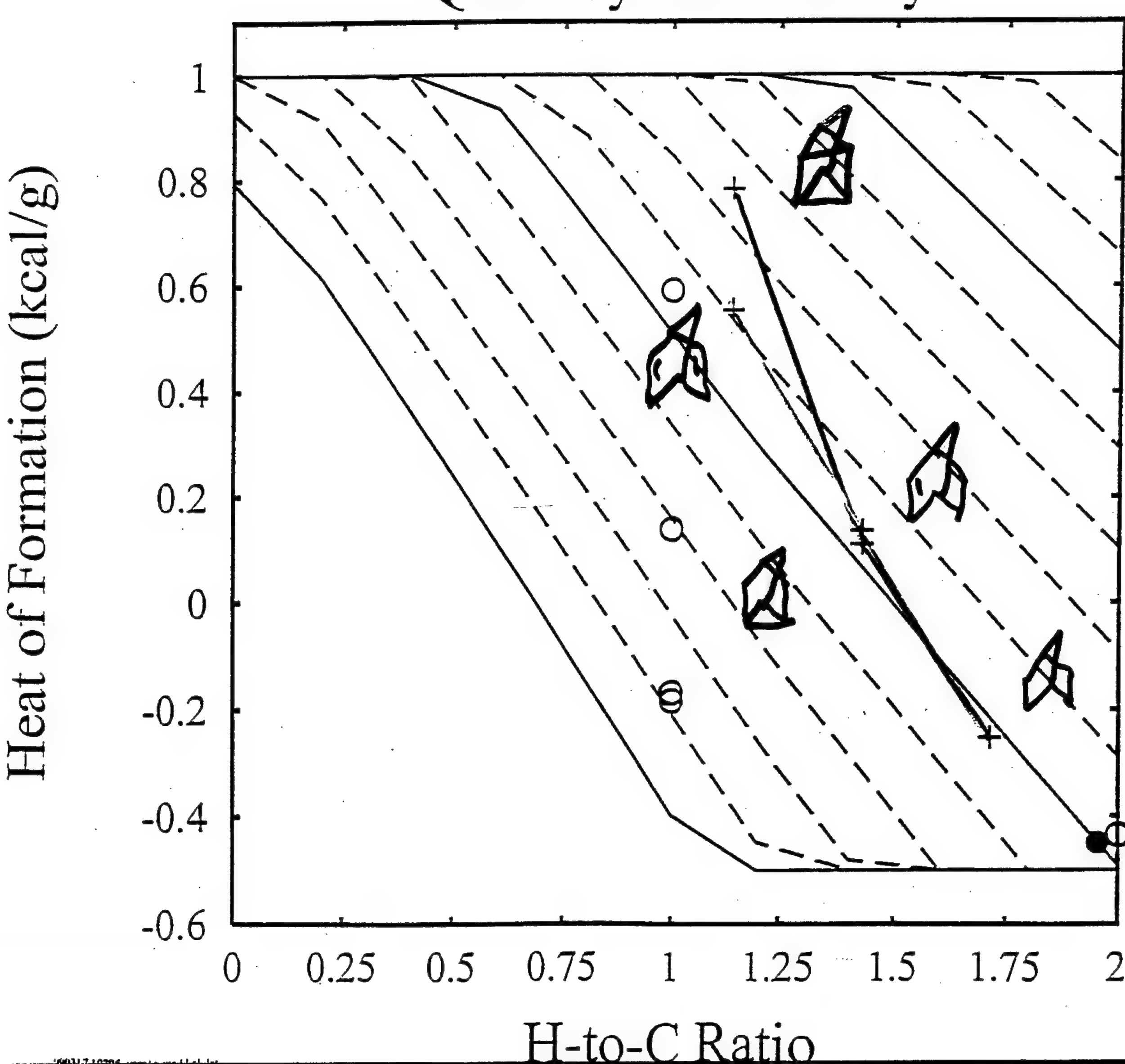
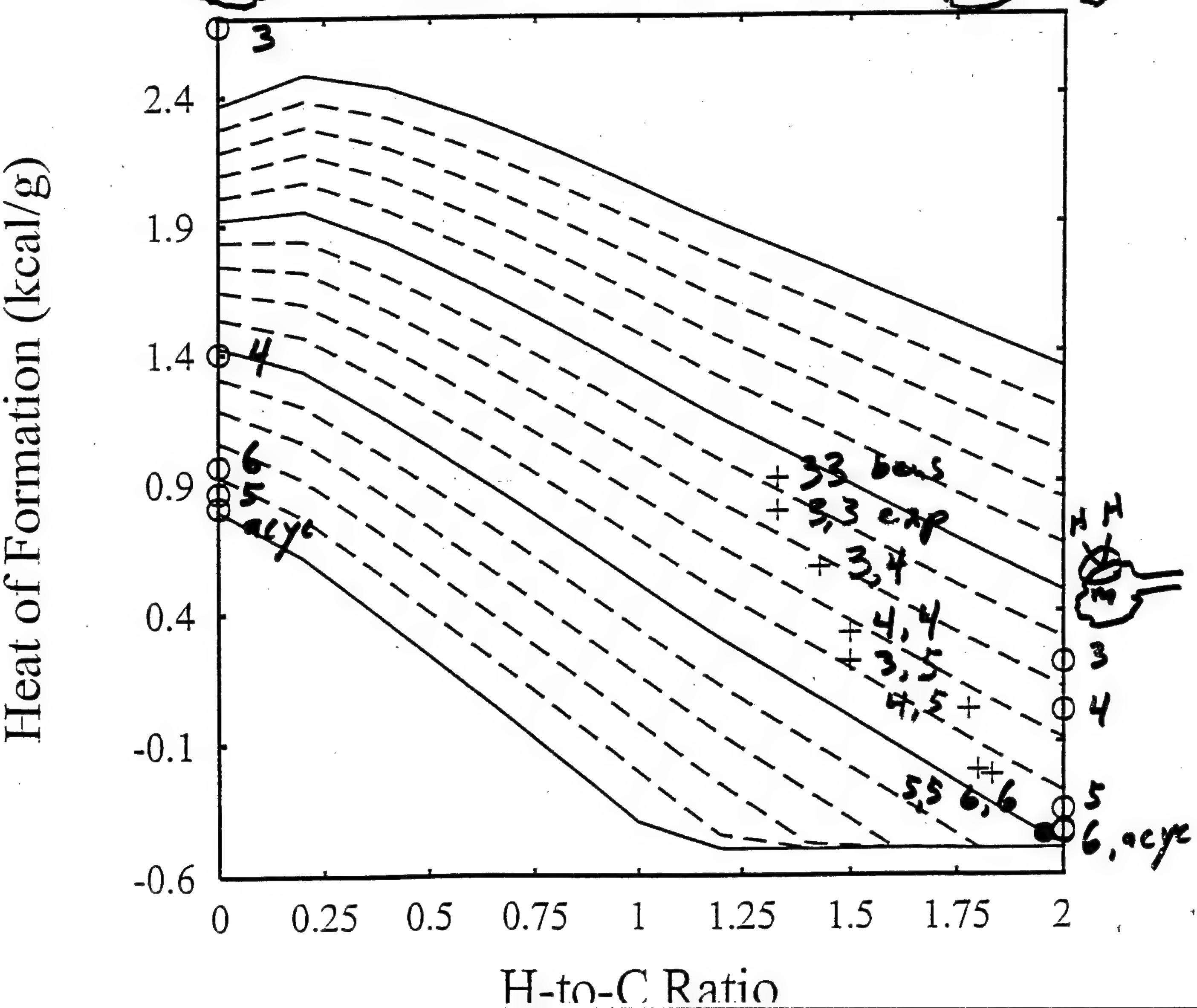
Liquid, Sea-Level Hydrocarbon Performance
Cycloalkenes



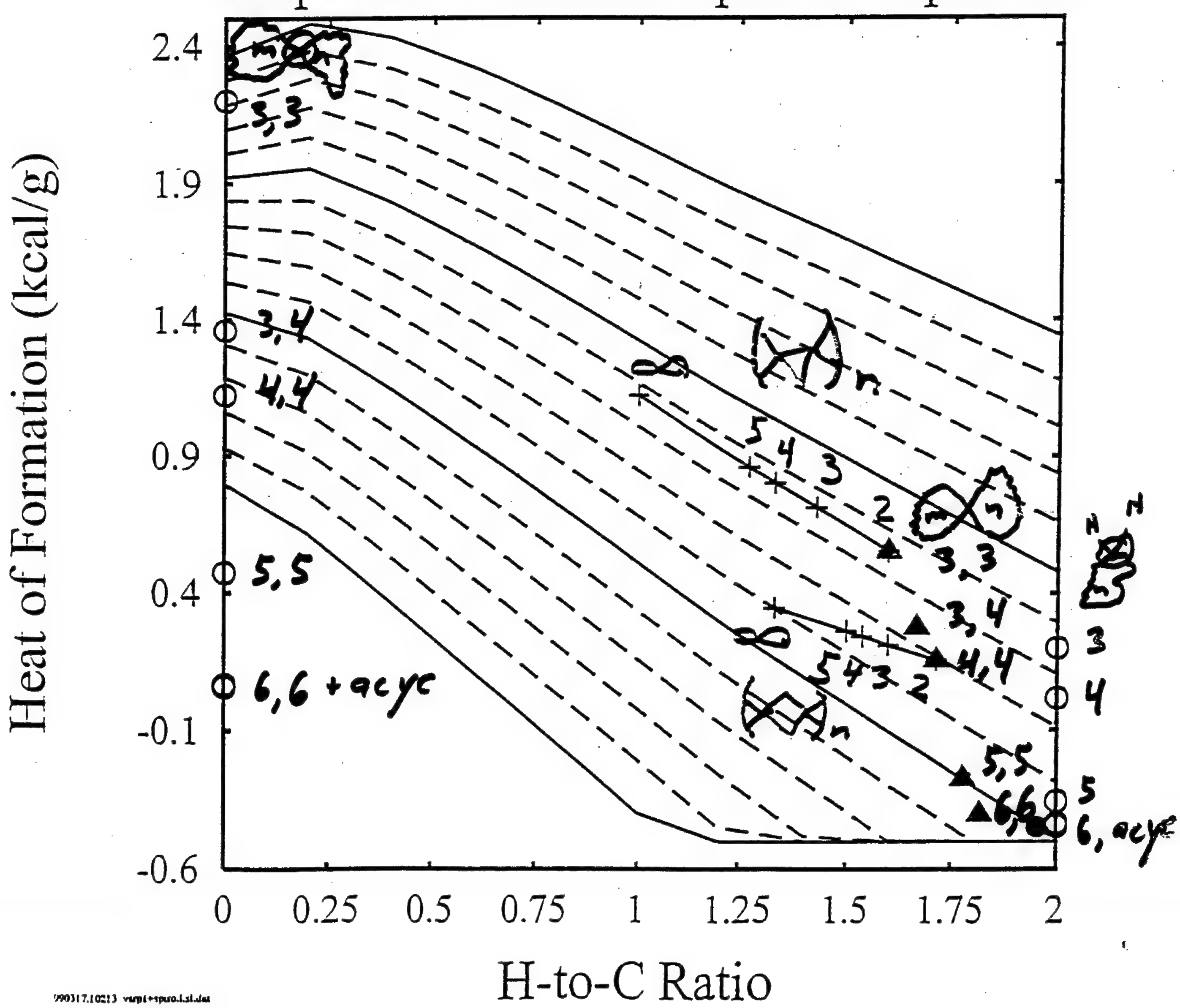
Liquid, Sea-Level Hydrocarbon Performance
Quadricyclane Family



Liquid, Sea-Level Hydrocarbon Performance
Double-Bow Molecules



Liquid, Sea-Level Hydrocarbon Performance
Simple and Catenated Spiro Compounds



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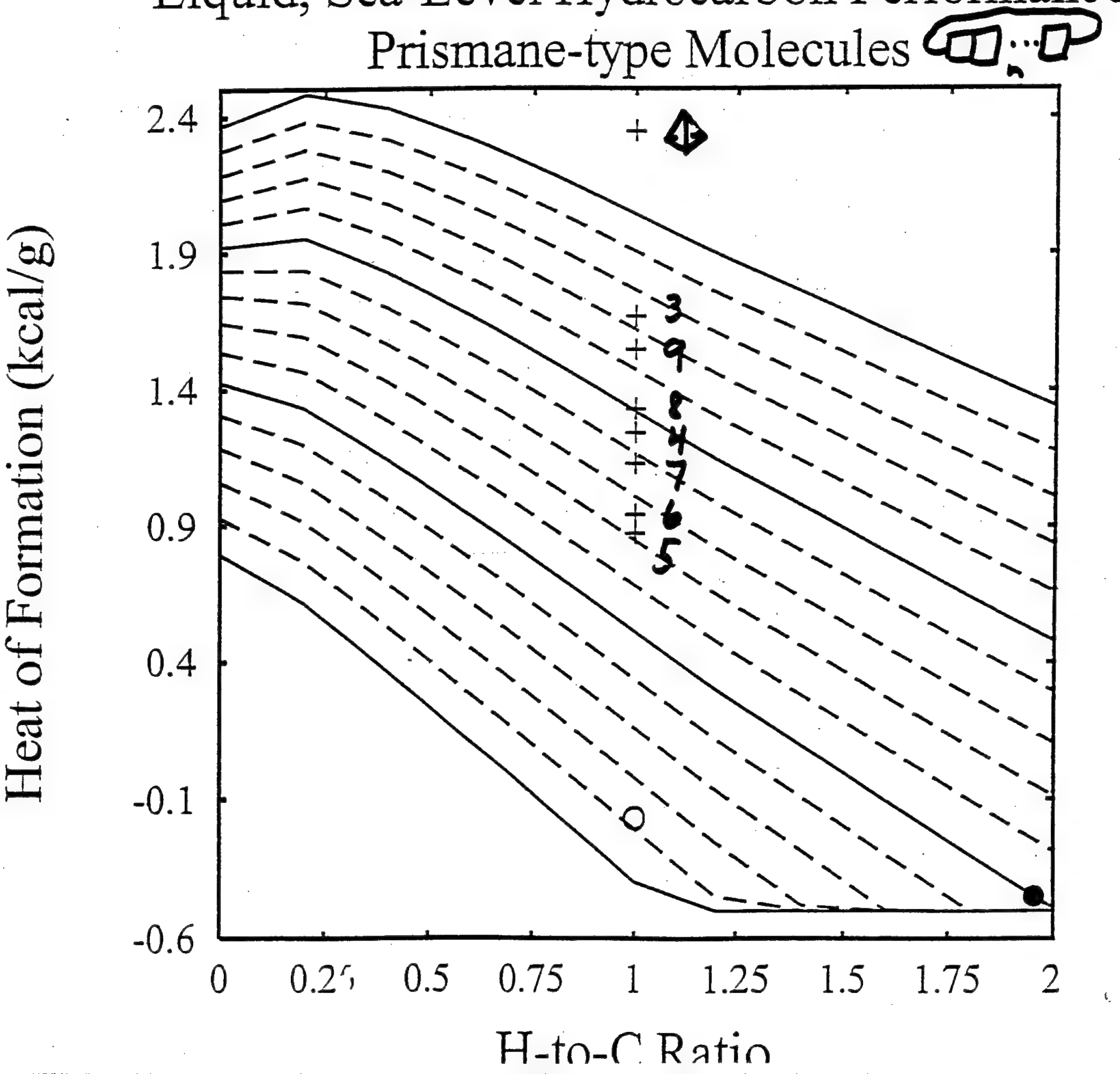
Liquid, Sea-Level Hydrocarbon Performance
Prismane-type Molecules



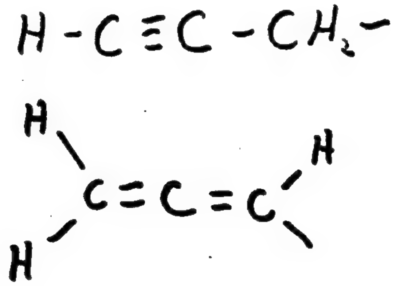
“Benson-Group” Specific Impulse–

Additional Approximation: Benson-Group *Gedanken* Rocket

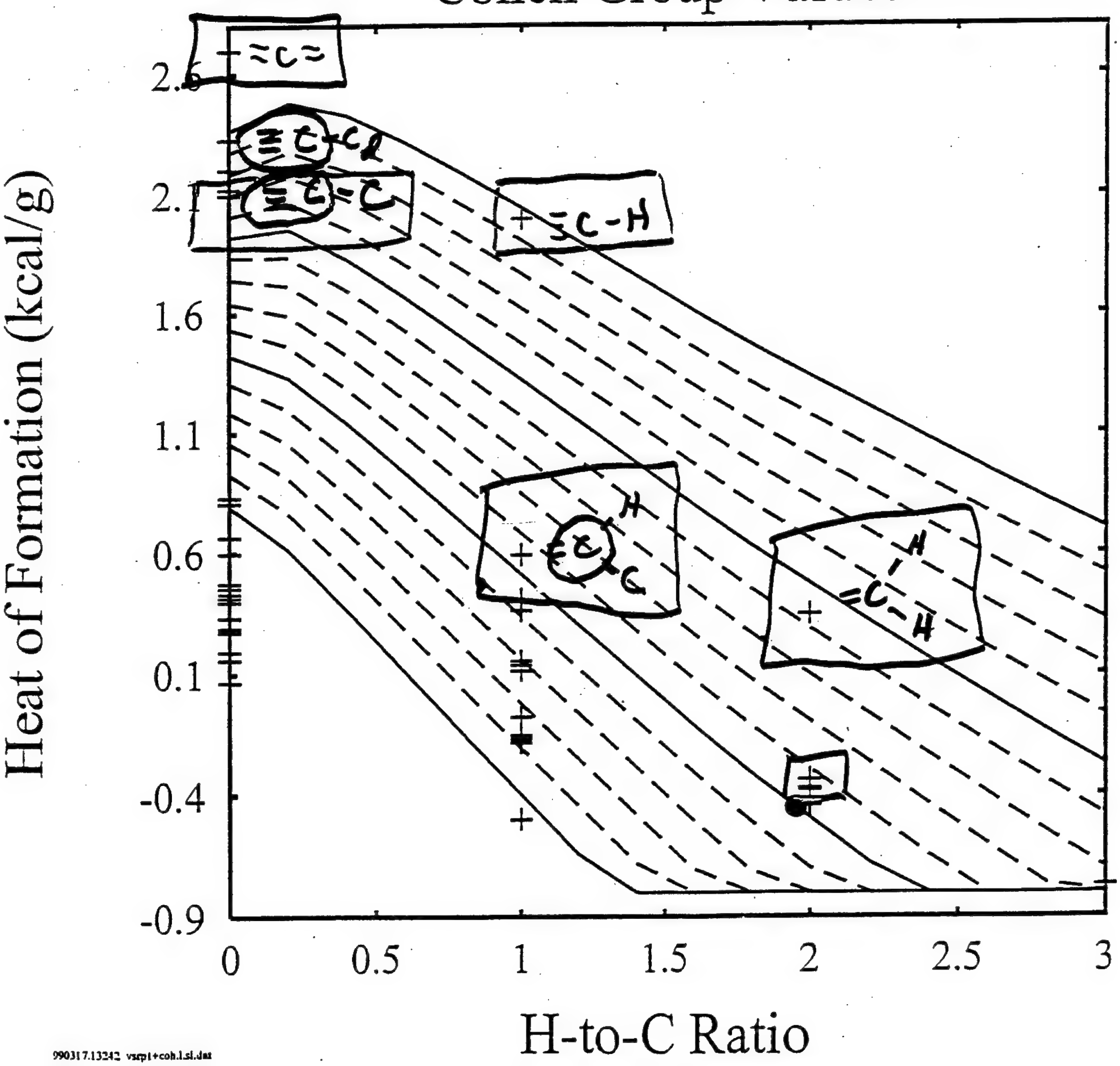
$$(I_{sp})_{opt} \approx \sum_{\substack{i \\ \text{groups}}} \frac{m_i}{m_{tot}} (I_{sp,i})_{opt}$$

$\frac{m_i}{m_{tot}}$–group mass fraction

$(I_{sp,i})_{opt}$–optimized specific impulse for the chemical group, alone



Liquid, Sea-Level Hydrocarbon Performance
Cohen Group Values



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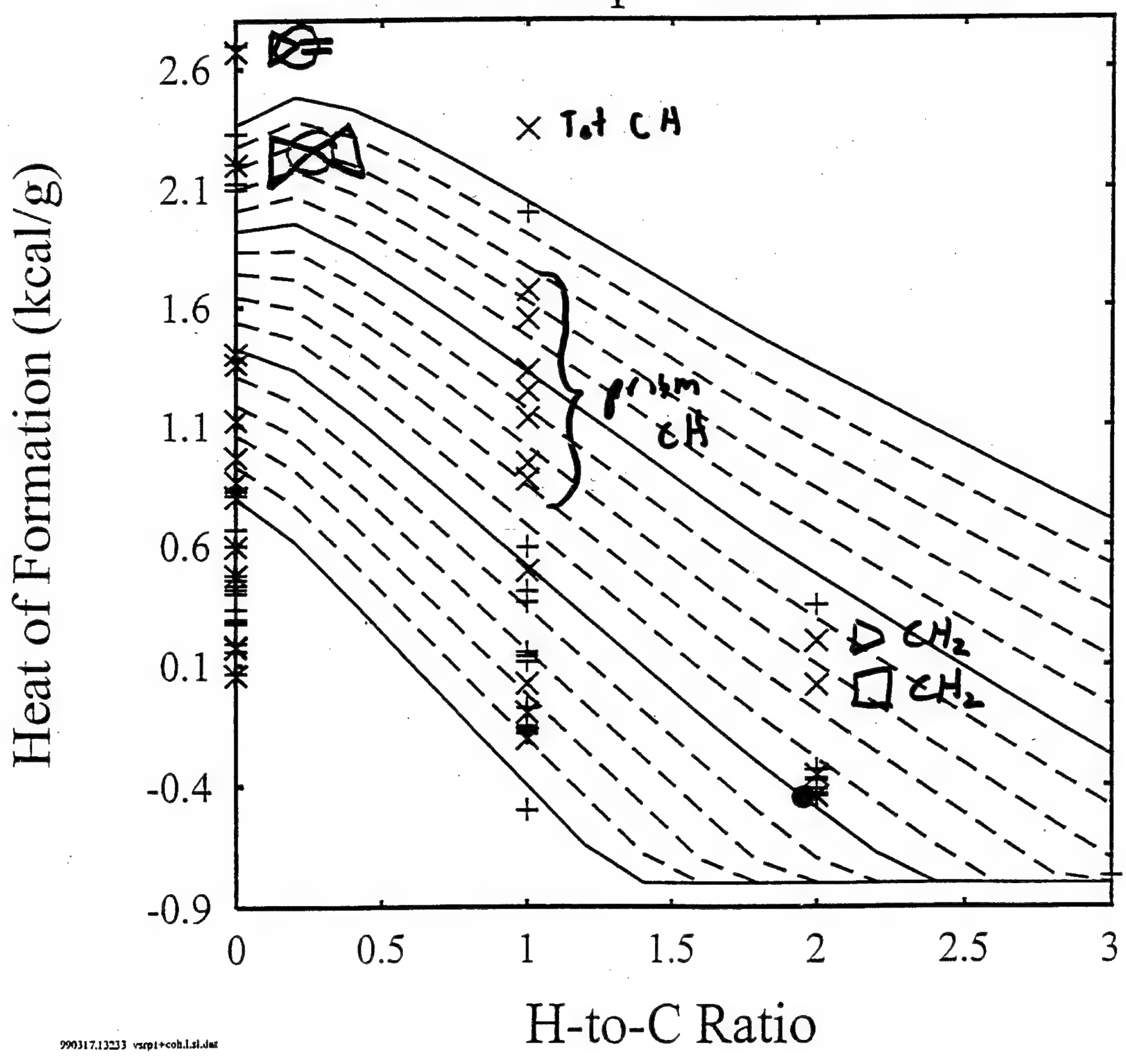
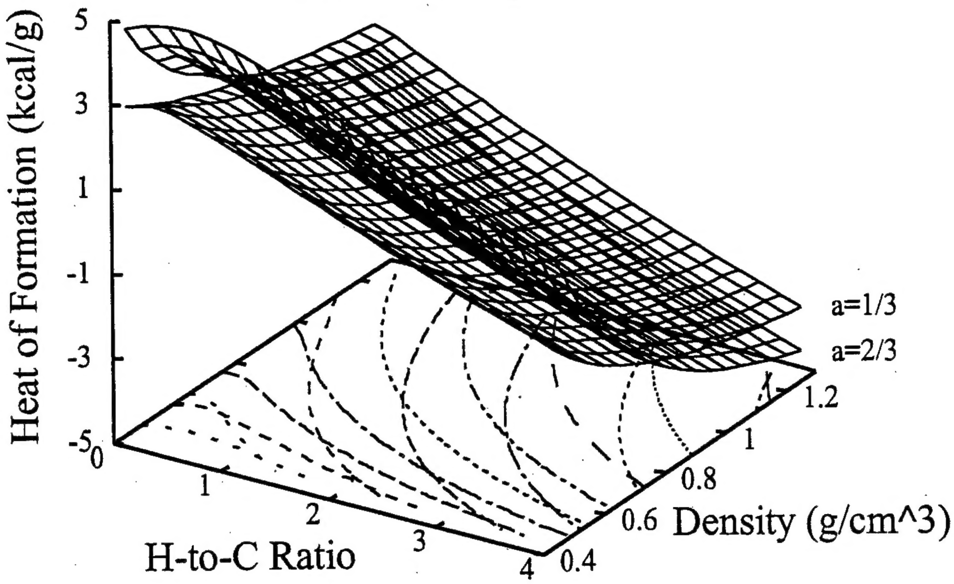
Liquid, Sea-Level Hydrocarbon Performance
Cohen Group Values + Extras



Effects of Fuel Density–

Optimium Density I_{sp} vs. LOX
Sea-Level Expansion



Summary and Future Directions–

- Specific ΔH_f, $r(\frac{H}{C})$, and fuel density, alone, determine model, LOX-optimized rocket performance of hydrocarbon fuels
- Performance trade-offs among these parameters have been quantified and illustrated for ready reference
- Hydrocarbon fuels can be sought among known molecules in the parameterized performance space herein described
- The "Benson specific impulse" provides at least a semi-quantitative guide in the search for new, unknown rocket fuels

- Other chemical systems may be explored using these insights (C,H,N; doped H_2)

Acknowledgments–

These calculations were performed on local IBM RISC workstations using a modified version of the Air-Force specific-impulse rocket code written by C. Selph, R. Hall, C. Beckman, R. Acree, T. Magee and others.